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COUPLED HYDROLOGIC AND GEOPHYSICAL INVERSION FOR CHARACTERIZATION OF NONAQUEOUS PHASE SOURCE ZONES

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Summary. *Concentration plume evolution and chemical persistence at chlorinated solvent contaminated sites are typically controlled by the presence of dense nonaqueous phase liquid (DNAPL) mass within a highly contaminated region or DNAPL source zone. Characterization of both the extent and structure of the source zone DNAPL mass distribution is, thus, of great importance to site assessment and successful remedial design. This paper provides an overview of ongoing research in our group designed to develop new approaches to DNAPL source zone characterization based on the joint inversion of hydrological and geophysical data. Hydrological data are obtained from three-dimensional (3D) simulations of DNAPL infiltration, entrapment, and subsequent rate-limited dissolution for a representative contaminant (PCE) under a range of geologic conditions. Electrical resistance tomography (ERT) is employed as the geophysical modality, where electrical resistivity is mapped to local saturations through an Archie's law expression. Simulated down gradient transect concentrations and cross-hole ERT measurements are then used, in conjunction with a shape-based inversion technique, to infer the source zone envelope (i.e, the region of space over which DNAPL saturation is nonzero), as well as the average saturation in this region. The potential performance of this approach for DNAPL source zone characterization is illustrated and discussed.*

1 INTRODUCTION

DNAPL source zone mass removal from contaminated aquifers has proven to be a challenging task. Over the last 25 years, significant research on mass recovery methods has demonstrated that no single technology will attain complete removal. However partial mass removal has the benefits of reducing longevity, concentration levels, and extent of the associated contaminant plume, as well as enhancing the efficiency of plume remediation technologies. To design effective mass removal strategies and evaluate site-specific benefits from partial mass removal, characterization of the extent and structure of the source zone DNAPL mass distribution is critical. Unfortunately existing methods for DNAPL characterization are both costly and intrusive, with attendant risks of DNAPL mobilization (e.g., partitioning interwell tracer tests). Here we present a new, relatively less intrusive approach to DNAPL source zone characterization that uses hydrological (down-gradient concentration) and geophysical (ERT) data. The two types of data are jointly inverted for DNAPL distribution characteristics, such as the geometry of the DNAPL contaminated region. The joint inversion technique employs a newly developed shape-based technique, the *parametric level set* method[1], that is capable of representing complex geometries and structures through relatively few parameters.

2 METHODS AND PROBLEM SETTING

Figure 1 illustrates the implementation of the joint inversion technique. A 3D multiphase immiscible flow simulator is first used to generate alternative realizations of source zone DNAPL mass distribution after contaminant release. A 3D flow and transport model, modified to incorporate rate-limited dissolution, is then used to compute contaminant concentrations within a down gradient transect, associated with a specific source zone saturation distribution and time. ERT is employed as the geophysical modality. Electrical potentials are obtained over arrays of electrodes on boreholes positioned cross gradient to the groundwater flow direction and on the earth's surface.

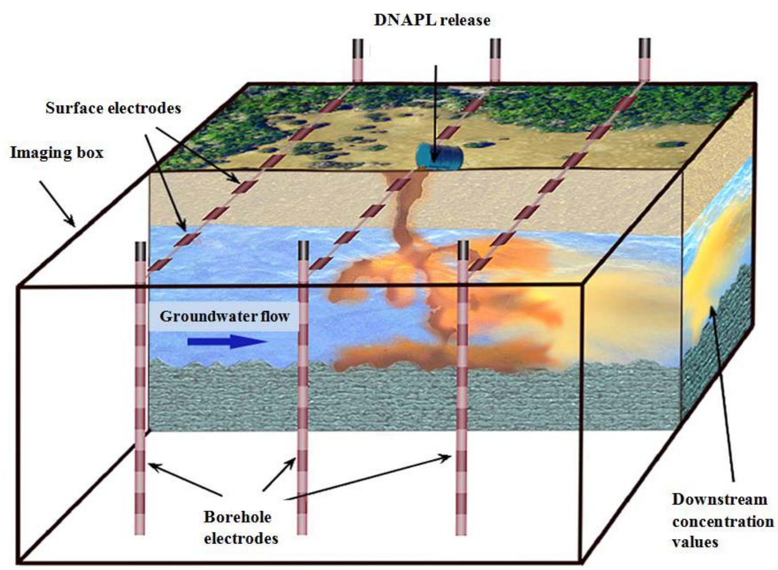

Figure 1: Implementation of the joint inversion technique

The inverse problem associated with the hydrological modality uses the down-gradient concentration data to invert for DNAPL saturation values, while the inverse problem associated with the geophysical modality inverts electrical data for the electrical conductivity distribution in the imaging domain. To relate the two modalities, a form of Archie's law[2] is employed to link the electrical properties of the medium to the saturation distribution. The ultimate goal of this inversion is to extract the geometry of the source zone region, along with a low order characterization of the spatial variability within the region of contamination.

2.1 Infiltration and dissolution of DNAPL

Simulation of DNAPL infiltration and subsequent mass dissolution in the saturated zone follows the methods outlined in[3,4]. Briefly, hysteretic infiltration and entrapment simulations were performed using the University of Texas Chemical Compositional Simulator (UTCHEM 9.0)[5]. Natural gradient dissolution simulations were obtained by means of a modified version of the modular three-dimensional transport simulator (MT3D)[6], which uses the Powers *et al.*[7] mass transfer correlation. Model hydrogeologic parameters were based on permeability realizations from a contaminated aquifer in Oscoda, Michigan (Bachman Road site), which consisted of relatively homogeneous glacial outwash sands[8]. Matrix properties of the permeability realizations originally developed by Lemke *et al.*,[9] were modified by varying the correlation length (integral scale), to encompass a range of geologic conditions.

2.2 Electrical resistance tomography

The ERT model is based on insertion of electrical current into a medium and measuring the electrical potential at the periphery of the medium to analyze the electrical conductivity distribution throughout the medium[10]. Based upon the conductivity contrast between DNAPL and the surrounding groundwater, reconstruction of the conductivity values $\sigma(x)$ can be a means of characterizing the source zone. For the imaging domain (3D DNAPL infiltration simulation) Ω with the boundary $\partial\Omega$ the underlying forward model is

$$\nabla \cdot \big(\sigma(x)\nabla u(x)\big) = j(x) \qquad \text{in } \Omega \tag{1}$$

$$\frac{\partial u}{\partial v} + \alpha u = 0 \qquad \text{on } \partial\Omega \tag{2}$$

Here u is the electrical potential and j is the current source. Regarding the boundary condition (2), $\partial u/\partial v$ denotes the normal component of the gradient of u on $\partial\Omega$. The function $\alpha(x)$ is defined on the boundary $\partial\Omega$, taking zero values on the air interface and appropriately chosen to model infinite half space for the remaining boundaries[11].

The petro-physical relationship that links the DNAPL conductivity values σ_n with the corresponding saturation values s_n is an Archie's law[2] expression:

$$\sigma_n = a\,\sigma_0 \varphi^p (1 - s_n)^q \tag{3}$$

where σ_0 is the non-saturated water conductivity, φ is the porosity of the medium, s_n is the DNAPL saturation and a, p and q are fitting parameters.

2.3 Parametric level set method

The standard inversion approach to this problem would involve the discretization of the imaging domain into a dense grid of pixels and inversion for the saturation values associated with each pixel. This approach results in a highly ill-posed inverse problem that is further complicated by the need to choose suitable regularization and associated regularization parameter(s). Here a more geometric approach to the problem is considered, based on level set concepts[12], that is better suited both to the limited information content in the data and the ultimate objective of the problem; i.e., characterizing the region of the subsurface contaminated by DNAPL. In a level set model the DNAPL saturation is represented as $s_n(x) = s(x)H\big(\psi(x)\big)$ where $H(.)$ is the Heaviside step function and $s(x)$ is a low order texture representation for the DNAPL distribution within the source zone. In the inverse problem, $H(.)$ is usually replaced by a smooth approximation. In the simplest case $s(x)$ can be considered as a scalar value representing the average DNAPL saturation in the source zone. In the course of inversion, an initial function $\psi^{(0)}$ is deformed to eventually reach a state such that its zero level set represents the true boundary. Although this approach is topologically flexible (i.e., requires no *a priori* assumption about the number of connected components in the domain) and better poses the problem by placing more emphasis on the geometry of the source zone, it still requires discretizing ψ in the whole imaging domain. To address this issue the parametric level set (PaLS) approach presented in[1] is employed, where the level set function is parameterized as $\psi(x) = \sum_{i=1}^{N} \alpha_i \phi(\|\beta_i(x - \chi_i)\|)$. Here ϕ is chosen to be a radial basis function and the quantities α_i, β_i and χ_i, known as the PaLS parameters, are the unknowns to be determined through the inverse processing. The value of N is intended to be much less than the number of pixels in a discretization approach. The low dimensionality of the PaLS problem avoids the need to apply regularization techniques and allows the use of Newton techniques for the minimization associated with the inverse problem.

2.4 Joint inversion

Consider $M_H(.)$ to be the full hydrological model linking DNAPL saturation values to downstream concentration observations d_H and $M_E(.)$ the electrical model that relates the conductivity values to electric potential measurements d_E. The electrical conductivity and saturation values are linked through the petro-physical relation $\sigma_n = P(s_n)$. In the PaLS approach, the DNAPL saturation is parameterized as $s_n(x, \mu)$, where μ includes the PaLS parameters and probably some low order texture parameters. Thus, the inverse problem takes the form of a finite dimensional multi-objective minimization problem

$$\mu^* = \arg\min_{\mu} \begin{cases} \mathcal{F}_E(\mu) \\ \mathcal{F}_H(\mu), \end{cases} \qquad (4)$$

where

$$\mathcal{F}_E(\mu) = \frac{1}{2}\left\|M_E\left(P\big(s_n(x,\mu)\big)\right) - d_E\right\|^2 \tag{5}$$

and

$$\mathcal{F}_H(\mu) = \frac{1}{2}\left\|M_H\big(s_n(x,\mu)\big) - d_H\right\|^2 \tag{6}$$

One of the main solution strategies in multi-objective optimization problems is the scalarization approach. In the current application, a scalarized version of the multi-objective problem would be $\mathcal{F}_T(\mu) = \mathcal{F}_H(\mu) + \eta\mathcal{F}_E(\mu)$, where $\eta > 0$ is a scalar usually chosen at the beginning of the minimization to make the two cost terms comparable. In the context of DNAPL characterization, the rate-limited dissolution process is governed by the equilibrium concentration in water and is limited by the capacity of the aqueous phase. Thus, as DNAPL saturation values increase within the source region, the downstream concentration values eventually stop monotonically increasing. Therefore in reconstructing relatively high DNAPL values, the reduction rate of $\mathcal{F}_E(\mu)$ may become more significant than that of $\mathcal{F}_H(\mu)$ when approaching the minima, resulting in an unbalanced convergence. For this reason, a variant of the multi- objective minimization technique[13] was applied, where at every iteration of the minimization a convex min-max problem of the form (7) is solved to obtain a descent direction δ_d

$$\delta_d = \underset{\delta}{\operatorname{argmin}}\ \max\begin{cases}\delta^T\mathcal{J}_H(\mu) + \frac{1}{2}\delta^T\mathcal{H}_H(\mu)\delta \\ \delta^T\mathcal{J}_E(\mu) + \frac{1}{2}\delta^T\mathcal{H}_E(\mu)\delta\end{cases} \tag{7}$$

In (7), $\mathcal{J}$ and $\mathcal{H}$ represent the Jacobian and the Hessian of each model. Using this approach, δ_d is guaranteed to be simultaneously the descent direction of both $\mathcal{F}_E(\mu)$ and $\mathcal{F}_H(\mu)$. For the ERT case, $\mathcal{J}_E$ can be calculated using adjoint field methods[14]. For the hydrological model, a finite difference approximation can be applied to extract the elements of $\mathcal{J}_H$, which can be accomplished efficiently due to the low dimensionality of μ.

3 RESULTS

The performance of PaLS, along with the presented joint inversion scheme, in reconstructing a challenging and realistic source zone structure is illustrated in Figure 2. The DNAPL distribution, shown in Figure 2.a, is spatially inhomogeneous and, for the purpose of visualization, is here displayed using two iso-contours. The light green color corresponds to low saturation values of 1% and the dark brown color corresponds to the profile of high saturation values of 15%.

The sensor placement and configuration associated with the ERT problem is also shown in Figure 2.a. In total 130 sensors are placed on the periphery of the imaging domain. For these simulations, a total of 32 experiments were carried out. In every experiment two sensors provided the electrical current and the remaining sensors measured the corresponding electric potential. The sensors acting as current sources were placed on six boreholes. The sensors in the remaining four boreholes and the surface sensors only acted as measuring sensors in all the experiments. With respect to the hydrological modality, the ground water flow is assumed to be in the $+x$ direction (Figure 2.a). The concentration measurements were performed in the $x = x_{\max}$ transect.

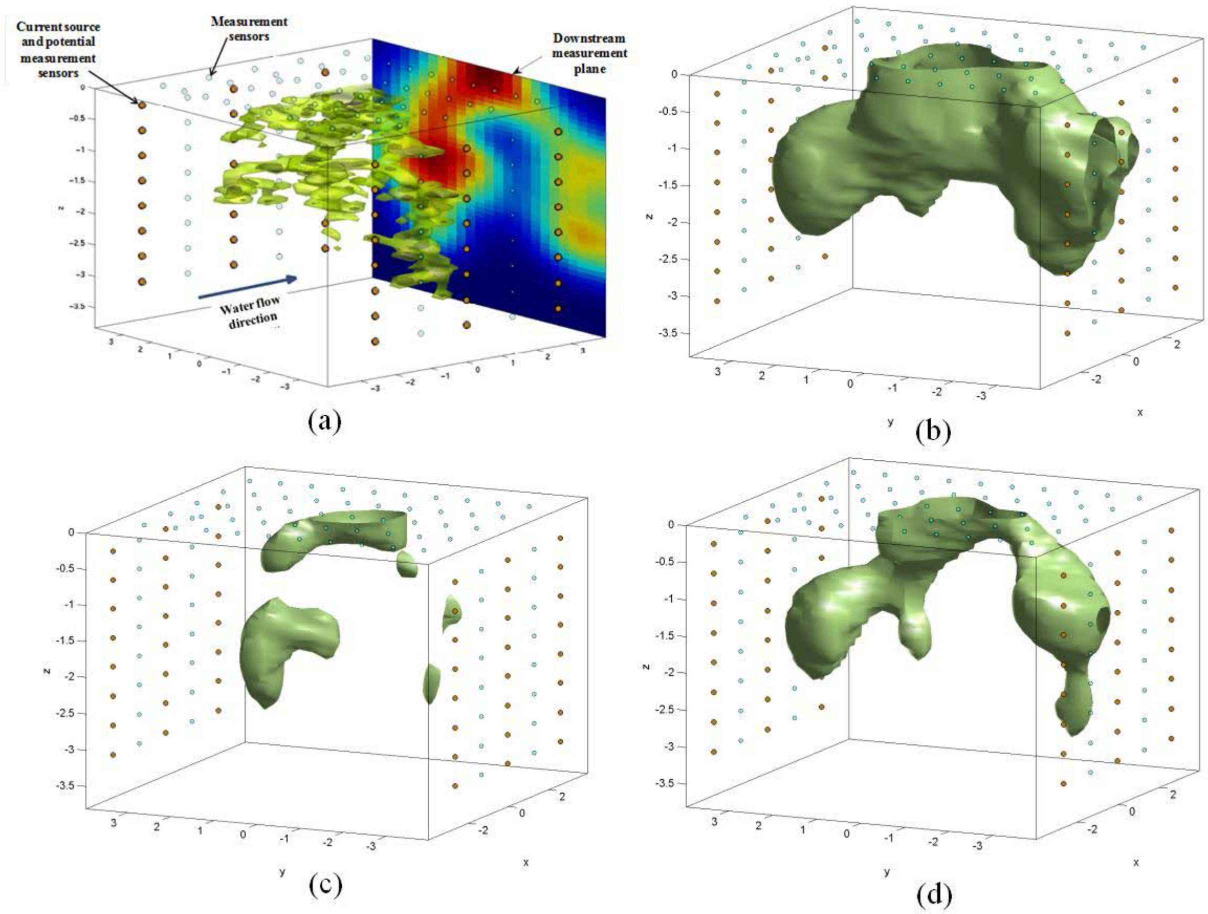

Figure 2: Results of the DNAPL reconstruction, (a) true DNAPL source zone with electrical and hydrological settings of the problem, (b) reconstruction using only ERT data, (c) reconstruction using only hydrologic data, and (d) reconstruction using newly developed joint inversion method

To initialize the PaLS parameters, we consider $s_n(x) = s(x)H(\psi(x,\mu))$ where $s(x) = s_0$ is a scalar representing the average DNAPL saturation within the source zone. This value is reconstructed along with the μ parameters. In this example, $N = 45$ basis functions were considered, with centers χ_i randomly chosen in the imaging domain and the other PaLS parameters were coarsely initiated resulting in an initial shape. Figure 2.b shows the result of an inversion using only the ERT data and Figure 2.c using only hydrologic data. The hydrologic inversion is clearly less successful due to the severe non-uniqueness that rate-limited dissolution imposes on the problem. Finally, Figure 2.d shows the result of jointly inverting electrical and hydrological data using the proposed joint inversion method. Comparing Figure 2.d with Figure 2.a, it is easily observable that this DNAPL reconstruction represents a very good match to the true DNAPL source zone envelope and preserves most of its important envelope details.

4 CONCLUSIONS

The overall approach presented in this paper is based upon the new parametric level set method, which enables rather complex geometries and structures to be described using relatively few parameters. Unlike conventional inversion methods, which rely on the inversion of the desired physical property values at a dense grid, this model-based approach significantly reduces the number of underlying parameters in the inversion. By posing the problem in this geometric framework, we are able to employ full 3D models as the basis for inversion for both the ERT and the multi-phase flow and transport. Additionally the newly developed PaLS method enables the joint inversion approach to have a denser data set corresponding to two different modalities (down gradient concentration and cross-hole ERT), an inversion that is almost impossible to conduct using traditional pixel-based techniques.

Compared to alternative approaches, such as partitioning interwell tracer tests, the combined use of ERT and down gradient concentration transect measurements for DNAPL source zone characterization is both less costly and less invasive, reducing the risk of contaminant mobilization. Prior to this research, however, the spatial complexity and low contrast and non-uniqueness issues associated with interpretation of these measurements greatly hampered their successful application in source zone characterization. The reconstruction results presented here are very promising and demonstrate that this new method is capable of handling inverse problems that use two different types of modalities of data sets, which makes it a well-suited, and computationally tractable, choice for complex inversion problems like characterization of DNAPL sources.

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